

Functional Bethe Ansatz Methods for the Open XXX Chain

Holger Frahm, Jan H. Grelik, Alexander Seel and Tobias Wirth

Institut für Theoretische Physik, Leibniz Universität Hannover,
Appelstr. 2, 30167 Hannover, Germany

Abstract

We study the spectrum of the integrable open XXX Heisenberg spin chain subject to non-diagonal boundary magnetic fields. The spectral problem for this model can be formulated in terms of functional equations obtained by separation of variables or, equivalently, from the fusion of transfer matrices. For generic boundary conditions the eigenvalues cannot be obtained from the solution of finitely many algebraic Bethe equations. Based on careful finite size studies of the analytic properties of the underlying hierarchy of transfer matrices we devise two approaches to analyze the functional equations. First we introduce a truncation method leading to Bethe type equations determining the energy spectrum of the spin chain. In a second approach the hierarchy of functional equations is mapped to an infinite system of non-linear integral equations of TBA type. The two schemes have complementary ranges of applicability and facilitate an efficient numerical analysis for a wide range of boundary parameters. Some data are presented on the finite size corrections to the energy of the state which evolves into the antiferromagnetic ground state in the limit of parallel boundary fields.

PACS: 02.30.Ik, 75.10.Pq

1 Introduction

The solution of the spectral problem for integrable models constructed within the framework of the Quantum Inverse Scattering method (QISM) is facilitated by a collection of various very powerful tools, commonly subsumed as Bethe ansatz methods. In Bethe's original work on the spin-1/2 Heisenberg chain [4] eigenfunctions were found by means of an ansatz for solutions of Schrödinger's equation in terms of scattering states of m magnons created from the completely polarized state as a reference which led to a system of coupled algebraic equations for m parameters. The roots of these Bethe equations correspond to particular eigenstates of the model in the m -magnon sector. Within the QISM this approach was put on an algebraic basis. For representations of a Yang-Baxter algebra the hamiltonian is identified as one member of a family of commuting operators generated by the transfer matrix. The eigenstates of this transfer matrix are obtained by the action of creation operators on the ferromagnetic reference state. The creation operators are functions of the roots of the Bethe equations.

This need for an eigenstate which is sufficiently simple to guess, however, limits the use of both the coordinate and the algebraic Bethe ansatz. For other cases, e.g. for models where the underlying symmetry is realized in a non-compact way without a highest weight state [5, 23] or situations where the $U(1)$ symmetry of the bulk is broken by interactions or boundary terms [18, 19] different approaches are needed: within the class of functional Bethe ansatz methods, e.g. Baxter's method of commuting transfer matrices, Separation of Variables (SoV), or the fusion algebra [3, 14, 25], relations between elements of the Yang-Baxter algebra are derived which eventually lead to functional equations for the eigenvalues of the transfer matrix. These relations have to be solved based on the analytic properties of the eigenvalues, e.g. distribution of zeros and poles, and their asymptotic behaviour. In certain cases this approach may lead to Bethe equations similar to those found within the coordinate or algebraic Bethe ansatz. In some cases where this is not possible, the functional relations have been brought to a form which allows to express them in terms of non-linear integral equations. From the analysis of these equations it has been possible to gain important insights into the properties of the ground state and low lying excitations as well as the thermodynamics for certain models, see e.g. [12].

In this paper we employ some of these functional methods to study the spectrum of the isotropic spin-1/2 Heisenberg chain with open boundary conditions where the symmetry of the bulk is broken due to non-parallel boundary magnetic fields. The model is given by the hamiltonian

$$\begin{aligned} \mathcal{H}_{XXX} = & \sum_{j=1}^{L-1} \left[\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \sigma_j^z \sigma_{j+1}^z \right] + L \\ & + \frac{i}{\alpha^-} \tanh \beta^- \sigma_1^z + \frac{i}{\alpha^- \operatorname{ch} \beta^-} \left(\operatorname{ch} \theta^- \sigma_1^x + i \operatorname{sh} \theta^- \sigma_1^y \right) \\ & + \frac{i}{\alpha^+} \tanh \beta^+ \sigma_L^z + \frac{i}{\alpha^+ \operatorname{ch} \beta^+} \left(\operatorname{ch} \theta^+ \sigma_L^x + i \operatorname{sh} \theta^+ \sigma_L^y \right) \quad , \end{aligned} \quad (1.1)$$

where σ_j^α , $\alpha = x, y, z$ denote the Pauli matrices acting on the space of states of a spin-1/2 at site j and α^\pm , β^\pm , θ^\pm parametrize the boundary fields acting on sites L and 1 respectively.

The hamiltonian (1.1) is obtained from a transfer matrix based on a representation of Sklyanin's reflection algebra [24] which extends the QISM to systems with open boundary conditions. Thereby the integrability of the model is established. At the same time, however, the fact that the ferromagnetically polarized state with all spins up is not an eigenstate of \mathcal{H}_{XXX} for generic boundary fields prevents the application of the coordinate or algebraic Bethe ansatz to the solution of the spectral problem. In a previous paper [9] we have used Sklyanin's Separation of Variables method to address this problem and have derived difference equations, so-called TQ -equations, which are satisfied by all eigenvalues of the transfer matrix. To access properties of the system in the thermodynamic limit $L \rightarrow \infty$, however, the characterization of the Q -functions appearing in these equations was incomplete. This is a familiar situation arising in the actual computation of spectral properties: to extract useful information from the Bethe equations one always needs some additional insights into the behaviour of their solutions as the system sizes varies, in particular for those corresponding to states with low energies or to the equilibrium state at finite temperature. This requirement appears to limit several other attempts to study spin chains with non-diagonal boundary terms based on e.g. representations of a q -Onsager algebra [2] or on an alternative use of the Yang-Baxter algebra due to Galleas [10]. Here we tackle this difficulty by identifying the analytical properties of the objects appearing in the TQ -equations and the related fusion hierarchy from finite size studies.

Our paper is organized as follows: in Section 2 we present a brief account of the construction of integrable boundary conditions within the QISM. We recall previous results obtained from SoV and by fusion of transfer matrices with higher dimensional auxiliary spaces. The spectral parameter in the TQ -equations derived within the SoV approach is restricted to a finite lattice of points which prevents the use of the functional methods for their solution. On the other hand, within the fusion procedure an equivalent TQ -equation with continuous arguments is obtained assuming that a certain limit of the fused transfer matrices exists for infinite dimensional auxiliary space (see also [21, 29]). Based on this equivalence we perform a finite size study of the analytical properties of the transfer matrix eigenvalues and of the Q -functions in Section 3. This allows one to derive a finite system of 'truncated' Bethe equations which we solve numerically for selected eigenstates of (1.1). In Section 4 we use our finite size data to rewrite the fusion hierarchy in terms of non-linear integral equations of TBA type whose solution determines one selected eigenstate of (1.1). The paper ends with a summary of our results and some concluding remarks.

2 Integrable Boundary Conditions

The construction of integrable systems involving boundaries within the QISM was initiated by Sklyanin [24]. It is valid for a general class of integrable systems characterized by an R -matrix of difference form $R(\lambda, \mu) = R(\lambda - \mu) \in \text{End}(V \otimes V)$ which satisfies the Yang-Baxter equation

$$R_{12}(\lambda - \mu) R_{13}(\lambda - \nu) R_{23}(\mu - \nu) = R_{23}(\mu - \nu) R_{13}(\lambda - \nu) R_{12}(\lambda - \mu) \quad . \quad (2.1)$$

The indices of R_{jk} denote the embedding where R acts non-trivially on the tensor product of vector spaces $V_1 \otimes V_2 \otimes V_3$. For the hamiltonian (1.1) we need the well-known 6-vertex model

solution

$$R(\lambda) = \begin{pmatrix} a(\lambda) & 0 & 0 & 0 \\ 0 & b(\lambda) & c(\lambda) & 0 \\ 0 & c(\lambda) & b(\lambda) & 0 \\ 0 & 0 & 0 & a(\lambda) \end{pmatrix}, \quad \begin{aligned} a(\lambda) &= \lambda + i \\ b(\lambda) &= \lambda \\ c(\lambda) &= i \end{aligned} \quad (2.2)$$

of the Yang-Baxter equation (2.1) with $V_j = \mathbb{C}^2$. Each solution $R(\lambda)$ fixes the structure constants of the related Yang-Baxter algebra

$$R_{12}(\lambda - \mu)T_1(\lambda)T_2(\mu) = T_2(\mu)T_1(\lambda)R_{12}(\lambda - \mu) \quad (2.3)$$

with generators $T^\alpha_\beta(\lambda)$, $\alpha, \beta = 1, 2$. $T_1(\lambda) = T(\lambda) \otimes I$, $T_2(\lambda) = I \otimes T(\lambda)$ are the embeddings of the monodromy matrix $T(\lambda)$ in the product of auxiliary spaces $V_1 \otimes V_2$, they satisfy the inversion formula

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \quad T^{-1}(\lambda) = \frac{1}{(d_q T)(\lambda - i/2)} \sigma^y T^t(\lambda - i) \sigma^y. \quad (2.4)$$

The scalar factor $(d_q T)(\lambda) = A(\lambda + i/2)D(\lambda - i/2) - B(\lambda + i/2)C(\lambda - i/2)$ is the central element of the Yang-Baxter algebra and is known as quantum determinant. The superscript t denotes a transposition and can be extended to the j th auxiliary space by t_j .

Sklyanin's construction of open spin chains is based on the representations of two algebras $\mathcal{U}^+(\lambda)$ and $\mathcal{U}^-(\lambda)$ defined by the relations

$$R_{12}(\lambda - \mu)\mathcal{U}_1^-(\lambda)R_{12}(\lambda + \mu - i)\mathcal{U}_2^-(\mu) = \mathcal{U}_2^-(\mu)R_{12}(\lambda + \mu - i)\mathcal{U}_1^-(\lambda)R_{12}(\lambda - \mu) \quad (2.5)$$

$$R_{12}(\mu - \lambda)\mathcal{U}_1^{+t_1}(\lambda)R_{12}(-\lambda - \mu - i)\mathcal{U}_2^{+t_2}(\mu) = \mathcal{U}_2^{+t_2}(\mu)R_{12}(-\lambda - \mu - i)\mathcal{U}_1^{+t_1}(\lambda)R_{12}(\mu - \lambda) \quad (2.6)$$

We shall call $\mathcal{U}^+(\lambda)$ and $\mathcal{U}^-(\lambda)$ right and left reflection algebras respectively. Considering their product in auxiliary space the trace

$$\tau(\lambda) = \text{tr} \mathcal{U}^+(\lambda) \mathcal{U}^-(\lambda) \quad (2.7)$$

defines the transfer matrix as the central object under consideration because it generates with $[\tau(\lambda), \tau(\mu)] = 0$ a commuting family of operators which can be simultaneously diagonalized.

The explicit construction of integrable open boundary conditions for models arising from the Yang-Baxter algebra with the R -matrix (2.2) starts with the 2×2 matrix

$$K(\lambda, \pm) = \frac{1}{\alpha^\pm \text{ch } \beta^\pm} \begin{pmatrix} \alpha^\pm \text{ch } \beta^\pm + \lambda \text{sh } \beta^\pm & \lambda e^{\theta^\pm} \\ \lambda e^{-\theta^\pm} & \alpha^\pm \text{ch } \beta^\pm - \lambda \text{sh } \beta^\pm \end{pmatrix} \quad (2.8)$$

independently found by [7, 11], considered in the rational limit [15] and used here in a parametrization introduced by Nepomechie [20]. It constitutes the known c -number representations $K^+(\lambda) = K(\lambda + i/2, +)$ and $K^-(\lambda) = K(\lambda - i/2, -)$ of the reflection algebras (2.5), (2.6) with the properties $\text{tr} K(\lambda, \pm) = 2$ and $K(0, \pm) = I_2$. Following Sklyanin we choose

$$\mathcal{U}^-(\lambda) = T(\lambda - i/2)K(\lambda - i/2, -)\sigma^y T^t(-\lambda - i/2)\sigma^y = \begin{pmatrix} \mathcal{A}^-(\lambda) & \mathcal{B}^-(\lambda) \\ \mathcal{C}^-(\lambda) & \mathcal{D}^-(\lambda) \end{pmatrix} \quad (2.9)$$

as representation incorporating the inversion formula (2.4). This leads to an explicit representation of the transfer matrix with normalization condition $\tau(i/2) = (d_q T)(-i/2)$ responsible for an additional factor of 1/2 in a similar decomposition of the right reflection algebra

$$\mathcal{U}^+(\lambda) = \frac{1}{2} K(\lambda + i/2, +) = \begin{pmatrix} \mathcal{A}^+(\lambda) & \mathcal{B}^+(\lambda) \\ \mathcal{C}^+(\lambda) & \mathcal{D}^+(\lambda) \end{pmatrix} . \quad (2.10)$$

Then the hamiltonian (1.1) is connected to the transfer matrix by $\mathcal{H}_{XXX} = i\partial \ln \tau(i/2)$.

2.1 Quantum Determinants

Analogously to the quantum determinant of the Yang-Baxter algebra there exists similar objects for the reflection algebras. Quantum determinants play a crucial role when applying functional methods to solve the spectral problem. For the left reflection algebra it is defined according to [24] reading with the projector P_{12}^- onto the singlet in $V_1 \otimes V_2$

$$(\Delta_q^- \mathcal{U})(\lambda) = \text{tr}_{12} P_{12}^- \mathcal{U}_1^-(\lambda - i/2) R_{12}(2\lambda - i) \mathcal{U}_2^-(\lambda + i/2) . \quad (2.11)$$

To express $(\Delta_q^- \mathcal{U})(\lambda)$ in terms of the generators $\mathcal{A}^-(\lambda)$, $\mathcal{B}^-(\lambda)$, $\mathcal{C}^-(\lambda)$ and $\mathcal{D}^-(\lambda)$ it is instructive to use the combinations

$$\tilde{\mathcal{D}}^-(\lambda) \equiv 2\lambda \mathcal{D}^-(\lambda) - i\mathcal{A}^-(\lambda), \quad \tilde{\mathcal{C}}^-(\lambda) \equiv (2\lambda + i)\mathcal{C}^-(\lambda) \quad (2.12)$$

borrowed from the algebraic Bethe ansatz. Then the suggestive form of the quantum determinant reads

$$(\Delta_q^- \mathcal{U})(\lambda) = \mathcal{A}^-(\lambda + i/2) \tilde{\mathcal{D}}^-(\lambda - i/2) - \mathcal{B}^-(\lambda + i/2) \tilde{\mathcal{C}}^-(\lambda - i/2) . \quad (2.13)$$

Thus in case of the c -number representation $K(\lambda - i/2, -)$ connected to the left reflection algebra $\mathcal{U}^-(\lambda)$ the relation

$$(\Delta_q^- K)(\lambda - i/2, -) = 2(\lambda - i) \det K(\lambda, -) = -2(\lambda - i) \frac{(\lambda - \alpha^-)(\lambda + \alpha^-)}{(\alpha^-)^2} \quad (2.14)$$

holds. Note that this connection is only valid for the shifted argument $\lambda - i/2$ because the arising expressions in (2.11) are no longer of difference form. As the quantum determinant respects co-multiplication, applying it to the full representation (2.9) of the left reflection algebra with the monodromy $T(\lambda)$ yields

$$(\Delta_q^- \mathcal{U})(\lambda) = (d_q T)(\lambda - i/2) (\Delta_q^- K)(\lambda - i/2, -) (d_q T)(-\lambda - i/2) . \quad (2.15)$$

The right reflection algebra can be treated in a similar way. We may leave with the suggestive form of the result

$$(\Delta_q^+ \mathcal{U})(\lambda) = \mathcal{D}^+(\lambda - i/2) \tilde{\mathcal{A}}^+(\lambda + i/2) - \mathcal{B}^+(\lambda - i/2) \tilde{\mathcal{C}}^+(\lambda + i/2) . \quad (2.16)$$

Again, we used some suitable combinations reading

$$\tilde{\mathcal{A}}^+(\lambda) \equiv -2\lambda \mathcal{A}^+(\lambda) - i\mathcal{D}^+(\lambda) , \quad \tilde{\mathcal{C}}^+(\lambda) \equiv (-2\lambda + i)\mathcal{C}^+(\lambda) \quad (2.17)$$

where in case of the c -number representation $K(\lambda + i/2, +)$ to the algebra $\mathcal{U}^+(\lambda)$ the quantum determinant takes the form

$$(\Delta_q^+ K)(\lambda + i/2, +) = -2(\lambda + i) \det K(\lambda, +) = 2(\lambda + i) \frac{(\lambda - \alpha^+)(\lambda + \alpha^+)}{(\alpha^+)^2} . \quad (2.18)$$

2.2 Separation of Variables

For diagonal boundary matrices the spectrum of the model has been obtained with the algebraic Bethe ansatz by action of the operators $\mathcal{B}^-(\lambda)$ on the completely polarized pseudo vacuum $|0\rangle$ [24]. In the case of generic boundary conditions, $|0\rangle$ is not an eigenstate of the transfer matrix and this approach is not possible. Instead one can follow Sklyanin's functional approach [25] based on the operator valued zeros \hat{x}_j of $\mathcal{B}^-(\lambda)$, $j = 1, \dots, L$. Studying representations of the reflection algebra on a space of symmetric functions of the eigenvalues x_j of these operators one obtains the TQ -equation for the eigenvalues Λ of the transfer matrix [9],

$$\Lambda(x_j) Q(x_j) = \frac{(-1)^L}{2x_j} \Delta^+(x_j) Q(x_j + i) + \frac{(-1)^L}{2x_j} \Delta^-(x_j) Q(x_j - i) \quad . \quad (2.19)$$

The coefficients $\Delta^\pm(\lambda)$ factorize the quantum determinant to the transfer matrix (2.7) according to $(\Delta_q^+ \mathcal{U})(\lambda) (\Delta_q^- \mathcal{U})(\lambda) = -\Delta^+(\lambda - i/2) \Delta^-(\lambda + i/2)$. Generalizing the transfer matrix to include inhomogeneous shifts parametrized by L lattice parameters s_j the eigenvalues of \hat{x}_j are found to be $x_j^\pm = s_j \pm i/2$ and the functions Δ^\pm are explicitly given as

$$\begin{aligned} \Delta^-(\lambda) &= (\lambda + i/2) \frac{(\lambda + \alpha^+ - i/2)(\lambda + \alpha^- - i/2)}{\alpha^+ \alpha^-} \prod_{\ell=1}^L (\lambda - s_\ell + i/2)(\lambda + s_\ell + i/2) \quad , \\ \Delta^+(\lambda) &= (\lambda - i/2) \frac{(\lambda - \alpha^+ + i/2)(\lambda - \alpha^- + i/2)}{\alpha^+ \alpha^-} \prod_{\ell=1}^L (\lambda - s_\ell - i/2)(\lambda + s_\ell - i/2) \quad . \end{aligned} \quad (2.20)$$

Note that only the diagonal parameters α^\pm of the boundary matrices enter in these equations. To obtain the spectrum for non-diagonal boundary fields corresponding to values of the parameters β^\pm and θ^\pm they have to be complemented with information on the asymptotic behaviour of $\Lambda(\lambda)$ at large $|\lambda| \gg 1$: from the construction of the transfer matrix one easily obtains [9]

$$\Lambda(\lambda) \sim \frac{(-1)^L \text{ch } \phi}{\alpha^+ \alpha^-} \lambda^{2L+2}, \quad \text{ch } \phi \equiv \frac{\text{sh } \beta^+ \text{sh } \beta^- + \text{ch}(\theta^+ - \theta^-)}{\text{ch } \beta^+ \text{ch } \beta^-} \quad . \quad (2.21)$$

Hence the parameter ϕ is sufficient to characterize the influence of the non-diagonal boundary fields. As a change in the sign of one α -parameter can be absorbed into the corresponding $\beta \rightarrow -\beta$ and $\theta \rightarrow \theta \pm i\pi$ with the mapping $\text{ch } \phi \rightarrow -\text{ch } \phi$ the complete parameter range of (1.1) is governed by $\text{ch } \phi > 0$ along with the cases $\alpha^+/i, \alpha^-/i > 0$ and $\alpha^-/i < 0 < \alpha^+/i$. As a simultaneous change $\alpha^\pm \rightarrow -\alpha^\pm$ formally reverses all spatial directions we do not need to consider the range $\alpha^+/i, \alpha^-/i < 0$.

The x_j^\pm are singular points of the difference equation (2.19), i.e. simple roots of the coefficients $\Delta^\pm(x_j^\pm) = 0$. Therefore, the Q -functions can be eliminated from (2.19) in favour of a functional equation for $\Lambda(x)$ valid on the discrete set $g = \{x_j^\pm\}$. It has been shown [9] that this equation yields the complete spectrum of the transfer matrix for small lattices. In the homogeneous limit $s_j \rightarrow s$ it becomes

$$\Lambda_g(s + i/2) \Lambda_g(s - i/2) = \frac{(s - \alpha^+)(s - \alpha^-)}{\alpha^+ \alpha^-} \frac{(s + \alpha^+)(s + \alpha^-)}{\alpha^+ \alpha^-} \frac{(s^2 + 1)^{2L+1}}{4s^2 + 1} \quad . \quad (2.22)$$

Here the subscript g emphasizes that (2.22) has been derived for the eigenvalue $\Lambda(\lambda)$ with arguments λ taken from the set g and therefore holds only up to terms which vanish as $(\lambda - s)^{2L+2}$. Still, neglecting this fact and taking s to be a continuous variable one can solve for $\partial \ln \Lambda_g(s)$ by Fourier transformation [9]. A particular state can be selected by imposing constraints on the analytical properties of Λ_g . For example the ground state eigenvalue has no zeros in the strip $|\operatorname{Im} z| < 1/2$. Evaluating the result at the point $i/2$ (c.f. (4.24)) this leads to the correct bulk and boundary contribution E_g to the ground state energy ($\psi(x)$ is the digamma function)

$$\begin{aligned} E_g \equiv i\partial \ln \Lambda_g(i/2) = & + \psi(|\alpha^+|/2) - \psi((|\alpha^+| + 1)/2) + 1/|\alpha^+| \\ & + \psi(|\alpha^-|/2) - \psi((|\alpha^-| + 1)/2) + 1/|\alpha^-| \\ & + \pi - 2 \ln 2 - 1 + (2 - 4 \ln 2)L \quad . \end{aligned} \quad (2.23)$$

Finite size corrections of order $\mathcal{O}(1/L)$ which would capture correlations between the two ends of the chain are beyond this approach.

2.3 Fusion Procedure

The so-called fusion procedure grants the possibility to easily obtain R -matrices and boundary matrices of higher dimensions obeying a Yang-Baxter or reflection equation respectively. In case of the R -matrix this procedure is applicable to the auxiliary, the quantum space, and even both. Furthermore the associated transfer matrices are not independent from each other but satisfy functional relations called fusion hierarchies.

An R -matrix of dimension $k/2$ in auxiliary space and a spin-1/2 representation in quantum space is given by e.g. [19] reading

$$R_{(1\dots k)\ell}(\lambda) = P_{1\dots k}^+ R_{1\ell}(\lambda) R_{2\ell}(\lambda + i) \cdots R_{k\ell}(\lambda + (k-1)i) P_{1\dots k}^+ \quad . \quad (2.24)$$

Here, the projector P^+ is defined as

$$P_{1\dots n}^+ = \frac{1}{n!} \sum_{\sigma \in \mathfrak{S}_n} P_\sigma \quad (2.25)$$

where the sum runs over all permutations $\sigma \in \mathfrak{S}_n$ of the symmetric group and P_σ is the permutation operator reordering the positions in the space $(\mathbb{C}^2)^{\otimes n}$ according to σ . The fused boundary matrices are defined in [31] following Mezincescu and Nepomechie [17] who carried out the first fusion step

$$K_{(12)}^+(\lambda) = P_{12}^+ K_2^+(\lambda + i/2) R_{12}(-2\lambda - 2i) K_1^+(\lambda - i/2) P_{12}^+ \quad (2.26)$$

similar to (2.24) explicitly. Utilizing the co-multiplication property one also finds

$$\mathcal{U}_{(12)}^-(\lambda) = P_{12}^+ \mathcal{U}_1^-(\lambda) R_{12}(2\lambda) \mathcal{U}_2^-(\lambda + i) P_{12}^+ \quad (2.27)$$

yielding a transfer matrix with a spin-1 auxiliary space $\tau_{(12)}(\lambda) \equiv \operatorname{tr}_{(12)} K_{(12)}^+(\lambda) \mathcal{U}_{(12)}^-(\lambda)$. With these definitions Mezincescu and Nepomechie [17] showed the fusion formula for the transfer matrix of the open boundary model

$$\tau_{(12)}(\lambda - i/2) = -(2\lambda - i)(2\lambda + i) \tau(\lambda - i/2) \tau(\lambda + i/2) - \frac{1}{4} (\Delta_q^+ K)(\lambda + i/2, +) (\Delta_q^- \mathcal{U})(\lambda) \quad (2.28)$$

depending on the quantum determinants of both reflection algebras and the original transfer matrix $\tau(\lambda)$ from (2.7). This result can be rewritten by absorbing the scalar prefactor in front of the τ 's into the definition of the fused transfer matrix giving

$$t_2(\lambda - i) = t_1(\lambda - i)t_1(\lambda) - \delta(\lambda) \quad , \quad \tau(\lambda + i/2) = \frac{(-1)^L}{\alpha^+ \alpha^-} t_1(\lambda) \quad (2.29)$$

with the scalar function $\delta(\lambda)$ on the RHS reading

$$\delta(\lambda) = \frac{(\lambda^2 + 1)^{2L+1}}{4\lambda^2 + 1} (\lambda - \alpha^+) (\lambda + \alpha^+) (\lambda - \alpha^-) (\lambda + \alpha^-) \quad . \quad (2.30)$$

Extending this procedure to higher dimensional auxiliary spaces [20,31] the arising transfer matrices t_k for integer k are finally related to each other through the fusion hierarchy

$$t_k(\lambda - i(k-1)) = t_{k-1}(\lambda - i(k-1))t_1(\lambda) - \delta(\lambda)t_{k-2}(\lambda - i(k-1)) \quad , \quad k = 2, 3, \dots \quad (2.31)$$

with $\delta(\lambda)$ given in (2.30) and $t_0(\lambda) \equiv 1$. Note that we do not have to distinguish between the transfer matrices $t_k(\lambda)$ and their eigenvalues because we are dealing with commuting quantities sharing a common system of eigenfunctions. Thus in the following we will use the notation t_k also for the eigenvalues. Again, the fusion hierarchy needs to be completed with the asymptotic behaviour $t_k(\lambda) \sim a_k \lambda^{(2L+2)k}$ of the eigenvalues of the fused transfer matrices: solving a recursion relation following from (2.31) and the asymptotic (2.21), (2.29) of the eigenvalue $\Lambda(\lambda)$ of $\tau(\lambda)$ as a starting value one obtains

$$t_k(\lambda) \sim a_k \lambda^{(2L+2)k} \quad , \quad a_k = \frac{1}{2^k} \frac{\text{sh}((k+1)\phi)}{\text{sh} \phi} \quad . \quad (2.32)$$

2.4 Equivalence of TQ-Equations

The fusion hierarchy (2.31) can formally be solved for the shifted eigenvalue $t_1(\lambda - i/2)$ related to spin-1/2 reading

$$t_1(\lambda - i/2) = \frac{t_k(\lambda + i/2 - i(k+1) + i)}{t_{k-1}(\lambda + i/2 - ik)} + \delta(\lambda - i/2) \frac{t_{k-2}(\lambda + i/2 - i(k-1) - i)}{t_{k-1}(\lambda + i/2 - ik)} \quad (2.33)$$

matching the general form of a TQ -equation [29]. Indeed, renormalization of the fused transfer matrices $t_k(\lambda)$ according to

$$t_k(\lambda) = a_k \left[\prod_{\ell=1}^{k-1} (\lambda + i\ell)^{2L+1} \prod_{\ell=1}^{k-1} (\lambda + i\ell + i/2)^{-1} \right] \tau_k(\lambda) \quad (2.34)$$

and assuming the limit $\lim_{k \rightarrow \infty} \tau_k(\lambda - ik - i/2) \equiv q(\lambda)$ to exist yields a difference equation

$$\begin{aligned} \Lambda(\lambda) q(\lambda) &= \frac{(-1)^L}{\alpha^+ \alpha^-} \frac{e^\phi}{2\lambda} (\lambda - i/2)^{2L+1} q(\lambda + i) \\ &+ \frac{(-1)^L}{\alpha^+ \alpha^-} \frac{e^{-\phi}}{2\lambda} (\lambda + i/2)^{2L+1} \left[\prod_{\sigma=\pm} (\lambda - i/2 - \alpha^\sigma) (\lambda - i/2 + \alpha^\sigma) \right] q(\lambda - i) \end{aligned} \quad (2.35)$$

which fixes the eigenvalue $\Lambda(\lambda)$ of $\tau(\lambda)$. With the transformation

$$q(\lambda) = (\mp 1)^{i\lambda} e^{i\lambda\phi} Q(\lambda) [\Gamma(-i\alpha^+ + 1/2 + i\lambda) \Gamma(-i\alpha^- + 1/2 + i\lambda)]^{-1} \quad (2.36)$$

we can absorb the exponential dependence on ϕ into $Q(\lambda)$ recovering the TQ -equation already obtained from the functional Bethe ansatz [9] reading

$$\begin{aligned} \pm \Lambda(\lambda) Q(\lambda) = & \frac{(-1)^L}{2\lambda\alpha^+\alpha^-} (\lambda - i/2)^{2L+1} (\lambda - \alpha^+ + i/2) (\lambda - \alpha^- + i/2) Q(\lambda + i) \\ & + \frac{(-1)^L}{2\lambda\alpha^+\alpha^-} (\lambda + i/2)^{2L+1} (\lambda + \alpha^+ - i/2) (\lambda + \alpha^- - i/2) Q(\lambda - i) \quad . \end{aligned} \quad (2.37)$$

In addition to the explicit appearance of α^\pm the boundary conditions enter this equation through the large- λ behaviour (2.21) of the eigenvalue $\Lambda(\lambda)$ and $\tau(\lambda)$ respectively.

For boundary parameters giving $\text{ch } \phi = \pm 1$ equation (2.37) can be solved by an even polynomial $Q(\lambda) = \prod_{j=1}^M (\lambda - \lambda_j)(\lambda + \lambda_j)$ where the λ_j are roots determined from the Bethe equations

$$\left(\frac{\lambda_j + i/2}{\lambda_j - i/2} \right)^{2L+1} \frac{\lambda_j + \alpha^+ - i/2}{\lambda_j - \alpha^+ + i/2} \frac{\lambda_j + \alpha^- - i/2}{\lambda_j - \alpha^- + i/2} = - \prod_{k=1}^M \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i} \frac{\lambda_j + \lambda_k + i}{\lambda_j + \lambda_k - i} \quad . \quad (2.38)$$

This case corresponds to boundary fields which can be dealt with by means of the algebraic Bethe ansatz. On the other hand, for $\text{ch } \phi \neq \pm 1$ no simple ansatz for $Q(\lambda)$ is known. However, for large $|\lambda|$ it has to grow exponentially $Q \sim \exp(-i\phi\lambda)$ according to (2.36).

3 Truncated Bethe Equations

After explicitly carrying out the large- k limit of the auxiliary space dimension for the transfer matrix t_k we are able to derive truncated Bethe equations in the non-diagonal boundary parameter range of $\phi \in \mathbb{R}$. Studying the root distributions of t_k for small system sizes yields information about the general root structure and it is possible to approximately treat the system with a finite number of zeros. With this knowledge on the analytical properties of the q -functions (2.35) leads to truncated Bethe equations. As a remark in the case of the XXZ model with diagonal boundaries and a special choice of boundary parameters the fusion hierarchy truncates exactly and the problem was already solved in [30] and [19] for non-diagonal boundaries respectively.

3.1 Iteration of the Fusion Equations

For systems with a few lattice sites ($L < 14$) the polynomial eigenvalues of the transfer matrix can be calculated explicitly either by exact formulas or numerical determination of the coefficients. Then the fusion hierarchy (2.31) can be used to compute the corresponding $\tau_k(\lambda)$ up to a specific fusion level k .

The roots of these functions $\tau_k(\lambda)$ are found¹ to be in the strip $-k - 1/2 \leq \text{Im } \lambda \leq 1/2$ and are symmetric with respect to the line $\text{Im } \lambda = -k/2$. As a consequence the zeros of

¹ This may not be true for all states. In cases where the ‘Bethe ansatz-part’ of the roots contains one or more string solutions the roots of $q(\lambda)$ may extend into the half plane $\text{Re } \lambda < 0$.

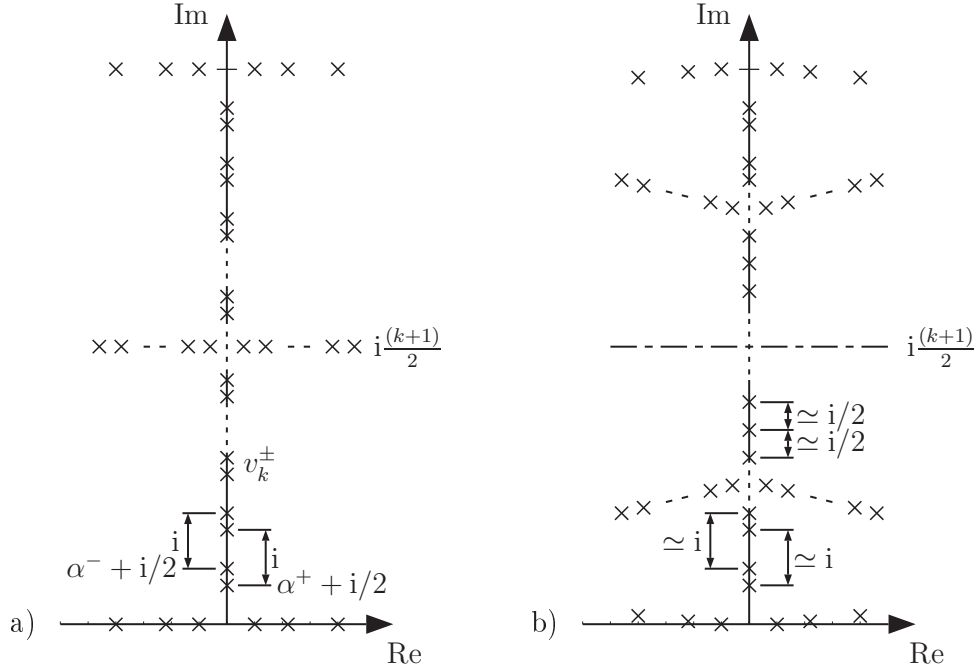


Figure 1: Typical root distributions for the A -state of $\tau_k(\lambda - ik - i/2)$ for an even system size L and $\text{Im } \alpha^-, \text{Im } \alpha^+ > 1/2$ (a) in the Bethe ansatz solvable case of $\text{ch } \phi = 1$ and (b) in the non-diagonal case of $\text{ch } \phi > 1$. Both distributions are symmetric to $\lambda = i(k+1)/2$.

$\tau_k(\lambda - ik - i/2)$ in (2.34), which are relevant in the limit $k \rightarrow \infty$ for the q -function, emerge in the region $0 \leq \text{Im } \lambda < (k+1)/2$ as denoted in Figure 1 for the Bethe ansatz solvable case (a) and for non-diagonal boundaries (b). Here we will concentrate on two distinguished states which we label by A and B : in the diagonal limit $\text{ch } \phi = \pm 1$ amenable to the algebraic Bethe ansatz the first state A turns into the singlet ground state of the antiferromagnetic chain whereas the B -state describes in this limit the fully magnetized state. Below we will study these states for boundary parameters $\text{Im } \alpha^\pm > 1/2$ which excludes boundary bound states.

For the Bethe ansatz solvable case in Figure 1a we observe in the A -state a distribution of zeros on the real axis, which are the known $2 \times L/2$ Bethe roots for this sector. In addition the q -function has roots on the imaginary axis which form a half-infinite lattice of spacing i starting at the points $\lambda = \alpha^\pm + i/2$. In the limit $k \rightarrow \infty$ this lattice becomes exact which allows to rewrite (2.35) as (2.37) with polynomial $Q(\lambda)$ as discussed above. The extra roots appearing on the symmetry line $\text{Im } \lambda = (k+1)/2$ for finite k can be neglected in the limit $k \rightarrow \infty$.

In cases with no Bethe ansatz the roots on the symmetry line move to branches in the complex plane which strongly depend on the asymptotic $\text{ch } \phi$. A typical root configuration for the A -state is shown in Figure 1b: we find that the number of roots forming these branches is fixed and their positions in the complex plane show only a slow variation with respect to the system size. The additional roots near the real axis evolve into the $2 \times L/2$ solutions of the Bethe equations (2.38) parametrizing the antiferromagnetic ground state in the limit $\text{ch } \phi \rightarrow 1$. The zeros v_k^\pm on the imaginary axis start from the points $\alpha^\pm + i/2$

with exponential accuracy (in L) and are approximately spaced by i as in the Bethe ansatz solvable case. However, at some imaginary point depending on the boundary parameters there is a crossover of the sequence v_k^\pm into a lattice of roots spaced by $i/2$. This lattice is approached with exponential accuracy which suggests to replace the sequence v_k^\pm beyond some (half) integer position iM by a compensating factor accounting for the asymptotics. This allows to treat the finitely many remaining roots with imaginary part $< M$ as in the treatise of the Bethe ansatz solvable case from above.

For the B -state a strong size dependence of the branches of extra roots is found which requires a more careful finite size analysis (see below).

3.2 Truncation

The analyticity of the transfer matrix eigenvalues (2.35) implies that the roots $q(\lambda_j) = 0$ have to satisfy an infinite hierarchy of Bethe equations

$$e^{-2\phi} \left(\frac{\lambda_j + i/2}{\lambda_j - i/2} \right)^{2L+1} \prod_{\sigma=\pm} (\lambda_j - i/2 - \alpha^\sigma)(\lambda_j - i/2 + \alpha^\sigma) = -\frac{q(\lambda_j + i)}{q(\lambda_j - i)} \quad (3.1)$$

for all $j \in \mathbb{N}$. In addition the restriction

$$e^{-2\phi}(i/2 - \alpha^+)(i/2 + \alpha^+)(i/2 - \alpha^-)(i/2 + \alpha^-) = \frac{q(i)}{q(-i)} \quad (3.2)$$

emerges from the residue at $\lambda = 0$ to vanish. Our findings on the asymptotic positions of the roots with $\text{Im} \lambda_j \gg 1$ (c.f. Figure 1b), i.e. by consecutive integers and half integers on the imaginary axis suggest us to explicitly deal only with the finite number N of zeros with $\text{Im} \lambda_j < M$ for some sufficiently large M depending on the boundary parameters α^\pm and ϕ . Within this approach the roots with $\text{Im} \lambda_j > M$ cancel (almost) perfectly in (2.35), i.e. we can replace

$$\begin{aligned} \frac{q(\lambda + i)}{q(\lambda)} &\rightarrow f(\lambda) \prod_{k=1}^N (\lambda - \lambda_k + i) \prod_{\ell=1}^{N-2} \frac{1}{\lambda - \lambda_\ell} \quad , \\ \frac{q(\lambda - i)}{q(\lambda)} &\rightarrow \frac{1}{f(\lambda - i)} \prod_{\ell=1}^{N-2} (\lambda - \lambda_\ell - i) \prod_{k=1}^N \frac{1}{\lambda - \lambda_k} \quad . \end{aligned} \quad (3.3)$$

The asymptotic behaviour (2.21) of the eigenvalue $\Lambda(\lambda)$ in the representation (2.35) requires $f(\lambda) \equiv 1$. As a result we obtain

$$\begin{aligned} \Lambda(\lambda) &= \frac{(-1)^L e^\phi}{\alpha^+ \alpha^- 2\lambda} (\lambda - i/2)^{2L+1} (\lambda - \lambda_N + i)(\lambda - \lambda_{N-1} + i) \prod_{k=1}^{N-2} \frac{\lambda - \lambda_k + i}{\lambda - \lambda_k} \\ &\quad + \frac{(-1)^L e^{-\phi}}{\alpha^+ \alpha^- 2\lambda} (\lambda + i/2)^{2L+1} \frac{\prod_{\sigma=\pm} (\lambda - i/2 - \alpha^\sigma)(\lambda - i/2 + \alpha^\sigma)}{(\lambda - \lambda_N)(\lambda - \lambda_{N-1})} \prod_{k=1}^{N-2} \frac{\lambda - \lambda_k - i}{\lambda - \lambda_k} \end{aligned} \quad (3.4)$$

from which we can derive truncated Bethe equations by the requirement of vanishing residues. The N remaining roots of $q(\lambda)$ have to satisfy the system

$$\begin{aligned} e^{-2\phi} \left(\frac{\lambda_j + i/2}{\lambda_j - i/2} \right)^{2L+1} &= \\ &= \frac{(\lambda_j - \lambda_{N-1})(\lambda_j - \lambda_{N-1} + i)(\lambda_j - \lambda_N)(\lambda_j - \lambda_N + i)}{(\lambda_j - i/2 - \alpha^+)(\lambda_j - i/2 + \alpha^+)(\lambda_j - i/2 - \alpha^-)(\lambda_j - i/2 + \alpha^-)} \prod_{\substack{k=1 \\ k \neq j}}^{N-2} \frac{\lambda_j - \lambda_k + i}{\lambda_j - \lambda_k - i} \end{aligned} \quad (3.5)$$

for $j = 1, \dots, N-2$. For $j = N-1, N$ the equations are ill-defined since the RHS vanishes identically. Note, however, that the analyticity of $\Lambda(\lambda)$ requires the residues of (3.4) at $\lambda = \lambda_N$ and $\lambda = \lambda_{N-1}$ to vanish. This condition can be met by setting $\lambda_{N-1} \equiv iM + i/2$ and $\lambda_N \equiv iM + i$ for the (half) integer M chosen for the truncation above as the zeros $\lambda_{N-2} \approx iM$ and $\lambda_{N-3} \approx iM - i/2$ are located close but not precisely on the asymptotic positions. As a test from the singularity of the eigenvalue Λ at $\lambda = 0$ the roots have to obey the restriction

$$e^{-2\phi} = \frac{\lambda_N(\lambda_N - i)\lambda_{N-1}(\lambda_{N-1} - i)}{(i/2 - \alpha^+)(i/2 + \alpha^+)(i/2 - \alpha^-)(i/2 + \alpha^-)} \prod_{k=1}^{N-2} \frac{\lambda_k - i}{\lambda_k + i} \quad (3.6)$$

Equations (3.5) can be solved numerically by Newton's algorithm. For the A -state this is possible due to the fact that the number and position of the roots forming the branch (c.f. Figure 1b) vary only slowly with respect to the system size for fixed boundaries. For the $2 \times L/2$ zeros near the real axis one can use the root distribution from the Bethe ansatz solvable case (2.38) as starting values. Doing so one obtains solutions for up to several thousand lattice sites which can be used to examine e.g. the finite size effects (c.f. Figure 4 in Section 4).

In the B -state the shape and position of the branches as well as the number of roots forming them strongly varies with the system size which prevents the derivation of truncated Bethe equations used above. However, a careful analysis of the arising root distributions leads to characteristic patterns as depicted in Figure 2 where we show typical results for α -parameters of equal sign.

3.3 Scope of Application

Clearly the method can also be applied to boundary bound states $0 < \text{Im } \alpha^\pm < 1/2$ with roots sticking to the points $i/2 - \alpha^\pm$ now being part of the parametrization (3.4) of the eigenvalue. For a plain overview of the terminology and parameter range see e.g. [22].

Note that the derivation of the equations (3.5) does not depend on the signs of the boundary parameters α^\pm : for boundary fields with opposite signs, $\text{sign}(\text{Im } \alpha^+) = -\text{sign}(\text{Im } \alpha^-)$, the root configuration corresponding to the A -state differs from the case above by the absence of the additional branches in the complex plane. For the B -state, branches as in Figure 2 are still present. Therefore, in both cases an analysis of the truncated Bethe equations is possible along the lines described before.

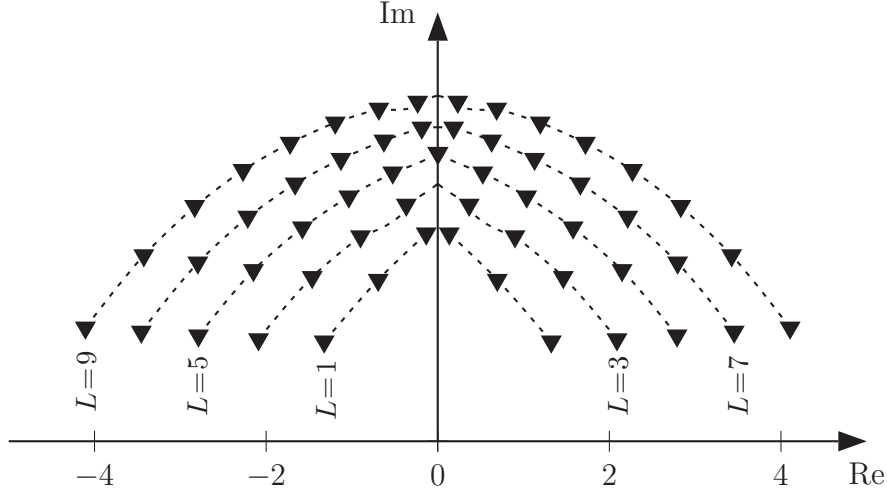


Figure 2: Root distributions for the B -state at $\alpha^\pm = 11i/3$ and $\text{ch } \phi = 11$. Zeros belonging to fixed lattice sizes $L = 1$ to $L = 9$ are each connected by a dashed line as a guidance for the eyes. The roots on the imaginary axis forming an asymptotic lattice of half integers are not displayed.

4 Y-System and Non-Linear Integral Equations

In order to directly capture the corrections to the bulk and boundary part (2.23) of the energy eigenvalue of the open spin chain one can use the methods of complex calculus to utilize the equivalent representation [14]

$$t_k(\lambda + i/2)t_k(\lambda - i/2) = t_{k-1}(\lambda + i/2)t_{k+1}(\lambda - i/2) + \prod_{\ell=1}^k \delta(\lambda - i/2 + i\ell) \quad (4.1)$$

of the fusion hierarchy (2.31). Following the standard scheme [16] one introduces the combination

$$y_2(\lambda) = \frac{t_2(\lambda - i)}{\delta(\lambda)} \quad (4.2)$$

being part of an infinite series $\{y_k\}$ related by functional relations. Once y_2 is known the eigenvalue of the underlying integrable model can be calculated from the lowest level

$$\Lambda(\lambda + i/2) \Lambda(\lambda - i/2) = \frac{\delta(\lambda)}{(\alpha^+ \alpha^-)^2} (1 + y_2(\lambda)) \quad (4.3)$$

of the fusion hierarchy (4.1) e.g. by Fourier techniques. Note the invariance of the functional equation (4.3) with respect to $\Lambda \rightarrow -\Lambda$ or $\alpha^\pm \rightarrow -\alpha^\pm$.

4.1 Y-System and Fourier Transformation

The aforementioned infinite system of functional relations is denoted as Y -system and can be derived for products of the transfer matrix eigenvalues. It is sometimes called the universal

form of the TBA-equations [16] and follows directly from the fusion hierarchy (4.1). By defining

$$y_k(\lambda) \equiv \frac{t_{k-2}(\lambda - i(k-2)/2)t_k(\lambda - ik/2)}{\prod_{\ell=1}^{k-1} \delta(\lambda - ik/2 + i\ell)} \quad (4.4)$$

and explicitly calculating $(1 + y_{k+1})(1 + y_{k-1})$ by making use of the fusion relation (4.1) one finds for integers k

$$y_k(\lambda - i/2) y_k(\lambda + i/2) = (1 + y_{k-1}(\lambda))(1 + y_{k+1}(\lambda)) \quad (4.5)$$

with $y_1 \equiv 0$. Note that a simultaneous scaling of $t_k(\lambda)$ and $\delta(\lambda)$ from (2.31)

$$t_1(\lambda) \rightarrow \frac{t_1(\lambda)}{p(\lambda)} \quad , \quad \delta(\lambda) \rightarrow \frac{\delta(\lambda)}{p(\lambda)p(\lambda - i)} \quad , \quad t_k(\lambda - i(k-1)) \rightarrow \frac{t_k(\lambda - i(k-1))}{\prod_{\ell=0}^{k-1} p(\lambda - i\ell)} \quad (4.6)$$

with any function $p(\lambda)$ leaves the Y -system (4.5) invariant. In view of this fact we choose $p(\lambda) = (2\lambda + i)^{-1}$ which allows to consider polynomial $\delta(\lambda)$ and $t_k(\lambda)$ rather than rational functions. Thus the zeros and poles of the y -functions can be identified with the zeros of $t_k(\lambda)$ and $\delta(\lambda)$, respectively. Taking the logarithmic derivative of the Y -system (4.5) and Fourier transforming

$$\widehat{f}(k) = \int_{-\infty}^{\infty} dx e^{-ikx} f(x) \quad , \quad f(x) = \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ikx} \widehat{f}(k) \quad (4.7)$$

the imaginary shifts occurring on the LHS can be removed leading to an infinite set of non-linear integral equations (NLIE) for the y -functions evaluated on the real line [27],

$$\begin{aligned} \ln y_2(x) &= d_2(x) + s * \ln(1 + y_3) \quad , \\ \ln y_k(x) &= d_k(x) + s * \ln(1 + y_{k-1}) + s * \ln(1 + y_{k+1}) \quad , \quad k > 2 \quad . \end{aligned} \quad (4.8)$$

Here $(s * f)$ denotes a convolution of f with the kernel

$$s(x) = \frac{1}{2 \operatorname{ch}(\pi x)} \quad , \quad \widehat{s}(k) = \frac{1}{2 \operatorname{ch}(k/2)} \quad . \quad (4.9)$$

As a consequence of the zeros and poles of the functions y_k their logarithmic derivatives are not analytic which produces the additional contributions $d_j(x)$ due to the residue theorem. The determination of these model-dependent driving terms is the challenging component of the problem. To reduce these terms we consider the toy equation

$$y(x + i/2)y(x - i/2) = F(x) \quad (4.10)$$

for $y(x)$ where $F(x)$ is given explicitly with constant asymptotic and the auxiliary condition $y(\pm\chi) = 0$ for some $\chi \in \{z \in \mathbb{C} | 0 \leq \operatorname{Im} z < 1/2\}$. Taking the logarithmic derivative one is led to

$$\int_{-\infty}^{\infty} dx e^{-ikx} \partial \ln y(x \pm i/2) = e^{\mp k/2} \left[\widehat{\partial \ln y}(k) \mp 2\pi i e^{\mp ik\chi} \right] \quad . \quad (4.11)$$

Switching to Fourier space we can solve (4.10) for $\widehat{\partial \ln y}(k)$ using the integral representation of the digamma function yielding

$$\int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{\text{sh}(\nu k/2)}{\text{ch}(k/2)} e^{ikx} = -\frac{1}{2\pi i} \partial_x \ln \left[\frac{\text{ch}(\pi x) - \sin(\pi \nu/2)}{\text{ch}(\pi x) + \sin(\pi \nu/2)} \right] . \quad (4.12)$$

Identifying $\nu = 1 - 2\chi/i$, inverse Fourier transforming and integration with respect to the variable x yields

$$\ln y(x) = C + \ln \left[\frac{\text{ch}(\pi x) - \cos(i\pi\chi)}{\text{ch}(\pi x) + \cos(i\pi\chi)} \right] + (s * \ln F)(x) \quad (4.13)$$

where the integration constant C can be recovered from the asymptotic condition of the initial equation (4.10).

Turning to the actual zeros of the y -functions we find that each $y_{k>2}$ has a double zero at $\lambda = 0$ whereas y_2 exhibits a $(2L + 2)$ -fold zero at $\lambda = 0$. To proceed we have to choose a particular state for which the transfer matrix t_1 and y_k do not contain further zeros in the strip $|\text{Im } z| < 1/2$ usually called hole-type solutions. Such a state exists for even lattice sites and opposite signs² of the boundary parameters α^\pm differing in their absolute values only by some finite amount (see below). This state is restricted to $\phi \in \mathbb{R}$, i.e. $\text{ch } \phi > 1$, and in the diagonal limit of $\phi \rightarrow 0$ it becomes the state with lowest energy in the sector of vanishing magnetization labeled A -state before. The corresponding driving terms (4.13) read for each double zero at $x = 0$ with $\chi \rightarrow 0$

$$\ln \left[\frac{\text{ch}(\pi x) - \cos(i\pi\chi)}{\text{ch}(\pi x) + \cos(i\pi\chi)} \right] \xrightarrow{\chi \rightarrow 0} \ln \tanh^2 |\pi x/2| \equiv \ln b_1^0(x) . \quad (4.14)$$

The poles of the y -functions can be treated in a similar way. Again, using (4.6) to scale the transfer matrix properly only the polynomial denominators, e.g. $\delta(\lambda + i/2)\delta(\lambda - i/2)$ for y_3 are responsible for the pole structure with respect to the boundary fields α^\pm . The multiple poles at $\lambda = 0$ are compensated by the transfer matrices. Already from the form of the arguments of each δ given in (2.30) it is clear that the positions of poles vary by $i/2$ for successive k and two poles of the same k differ by i . The general scheme is depicted in Figure 3. Thus using the parametrization $\alpha = i(n/2 + \alpha')$ with $n \in \mathbb{N}_0$ fixed and $0 < \alpha' < 1/2$ the function $y_k(\lambda)$ shows poles at $\lambda = \pm i\alpha'$ for indices $k \in \{n + 2\mathbb{N}\}$ and poles at $\lambda = \pm(i/2 - i\alpha')$ for indices $k \in \{n + 1 + 2\mathbb{N}\}$. The corresponding driving terms arise from (4.12) by inverting the sign on the RHS accounting for poles rather than zeros yielding negative logarithms of

$$h_c(x) \equiv \frac{\text{ch}(\pi x) - \cos(\pi\alpha')}{\text{ch}(\pi x) + \cos(\pi\alpha')} \quad \text{for } k \in \{n + 2\mathbb{N}\} \quad (4.15)$$

$$h_s(x) \equiv \frac{\text{ch}(\pi x) - \sin(\pi\alpha')}{\text{ch}(\pi x) + \sin(\pi\alpha')} \quad \text{for } k \in \{n + 1 + 2\mathbb{N}\} . \quad (4.16)$$

²Note that for α^\pm -parameters of equal sign and small k the branches in Figure 1b appear as unwanted hole-type solutions in the considered strip. The same holds in the parameter range $\phi \in i\mathbb{R}$ for any combination of the α -parameters.

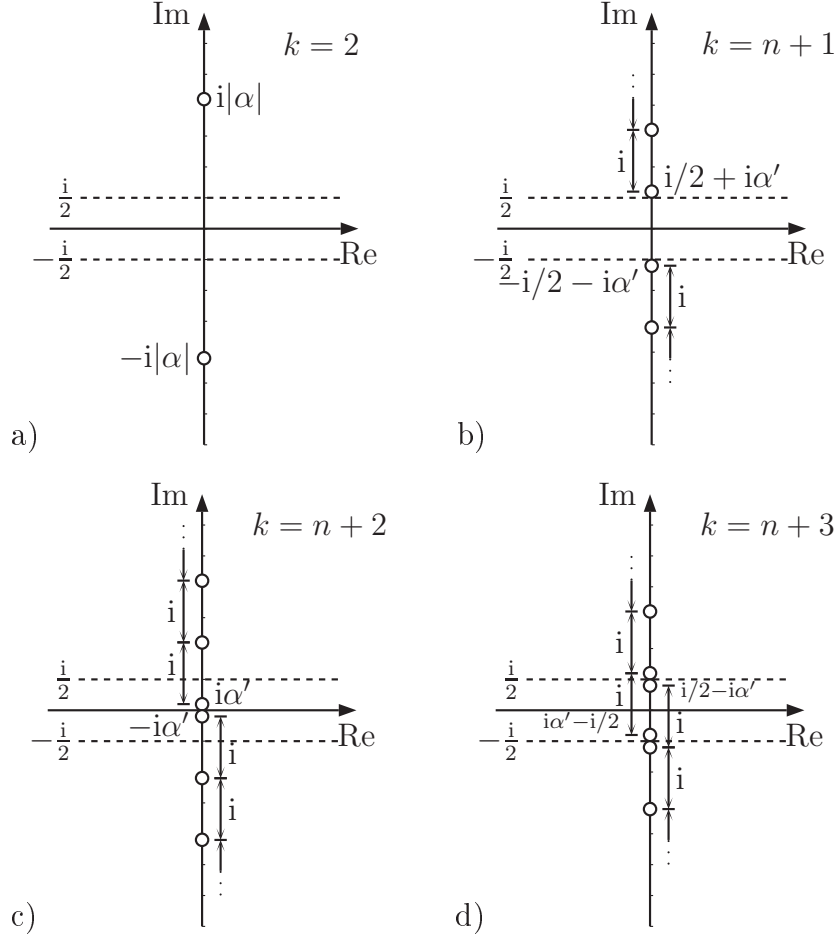


Figure 3: Exemplary position of poles (\circ) of y_k in the complex plane arising from one boundary field α for a) $k = 2$, b) $k = n + 1$, c) $k = n + 2$ and d) $k = n + 3$. With these examples all different cases of singularities inside the strip $|\operatorname{Im} \lambda| < 1/2$ are already considered.

Note that only the modulus of the parameter α enters and the terms h_c and h_s alternate for successive k . In summary a single zero at $\lambda = 0$ gives a driving term of $\ln \tanh |\pi x/2|$ and due to logarithmic derivative the multiplicity is only reflected in the integer prefactor. Rearranging all driving terms in matrix form

$$b_k^n(x) = \begin{pmatrix} & \begin{array}{c|cccc\cdots k} & 1 & 2 & 3 & 4 & \cdots & k \\ \hline 0 & \tanh^2 |\pi x/2| & h_c(x) & h_s(x) & h_c(x) & \cdots & \\ 1 & 1 & 1 & h_c(x) & h_s(x) & \cdots & \\ 2 & 1 & 1 & 1 & h_c(x) & \cdots & \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \\ n & & & & & & \end{array} \end{pmatrix} \quad (4.17)$$

allows us to write the non-linear integral equations in a compact form. For boundary parameters $\alpha^\pm = \pm i(n^\pm/2 + \alpha'_\pm)$ with $n^+ = n^- = n \in \mathbb{N}_0$ we find for an asymptotic condition

ch $\phi \geq 1$ of the transfer matrix the infinite set of equations

$$\begin{aligned} \ln y_2(x) &= (L+1) \ln b_1^0(x) - \ln b_2^{n^+}(x) - \ln b_2^{n^-}(x) + s * \ln(1 + y_3) \\ \ln y_k(x) &= \ln b_1^0(x) - \ln b_k^{n^+}(x) - \ln b_k^{n^-}(x) \\ &\quad + s * \ln(1 + y_{k-1}) + s * \ln(1 + y_{k+1}) \quad , \quad k > 2 \end{aligned} \quad (4.18)$$

for an even L . With the asymptotic condition $b_k^n(x) \rightarrow 1$ for $x \rightarrow \pm\infty$ no further integration constants have to be considered as the constant asymptotic

$$y_k \sim y_k^\infty = \frac{\text{sh}((k-1)\phi) \text{sh}((k+1)\phi)}{\text{sh}^2 \phi} \quad (4.19)$$

already satisfies the hierarchy (4.18) in the limit of $x \rightarrow \pm\infty$.

To solve an infinite system of equations such as (4.18) numerically a controlled scheme for its truncation is needed. In the standard TBA approach [28], e.g. for periodic boundary conditions, such an approximation can be based on the fact that (i) only the first few of the NLIE contain a non-zero driving term and (ii) the asymptotic solution (4.19) solves the NLIE without driving terms. Replacing $y_k(x)$ by this constant asymptotic for some k chosen sufficiently large one is left with a finite set of NLIE which can be solved numerically very efficiently.

In the case of open boundary conditions the NLIE contain driving terms for all levels k and therefore the asymptotics (4.19) determine only the large- x behaviour. Nevertheless, our numerical results using the constant asymptotic of y_k^∞ as an approximative limiting function seems to assure convergence of the system reasonably well. In the special cases of diagonal boundaries $\phi = 0$ we find that it is better to scale the constant asymptotic by the necessary driving terms in order to gain higher accuracy or use less equations without losing accuracy.

For asymptotic parameters $\phi \neq 0$ the constant solution (4.19) grows exponentially with k and numerical limitations are quickly reached restricting the method to ch $\phi = \mathcal{O}(1)$. The number of non-linear integral equations, necessary for decent accuracy, produces function values for which more sophisticated numerical treatment is needed. In principle, this simple approach which just uses the asymptotic as a limit function can be improved by considering solutions of (4.18) in the limit of $\max\{n^+, n^-\} \ll k$. It turns out, however, that this more sophisticated treatment of the asymptotics shown in Appendix A does not allow to reduce the number of NLIE substantially and that the restriction to ch $\phi = \mathcal{O}(1)$ prevails.

4.2 Energy Eigenvalue

Once the full hierarchy for $y_k(x)$ is solved the function $y_2(x)$ (and its analytical continuation) can be used to determine the polynomial eigenvalue $\Lambda(\lambda)$ of the transfer matrix. Identifying the quantum determinant $\delta(\lambda) = (\alpha^+ \alpha^-)^2 \Lambda_g(\lambda + i/2) \Lambda_g(\lambda - i/2)$ with (2.22) we see from the lowest level

$$\Lambda(\lambda + i/2) \Lambda(\lambda - i/2) = \Lambda_g(\lambda + i/2) \Lambda_g(\lambda - i/2) (1 + y_2(\lambda)) \quad (4.20)$$

of the fusion hierarchy that the corrections to bulk and boundary contributions [9] are contained in y_2 . The logarithmic derivative of the eigenvalue reads after simple manipulations

in Fourier space

$$\partial \ln \Lambda(x) = \partial \ln \Lambda_g(x) + \int_{-\infty}^{\infty} \frac{dk}{2\pi} \frac{e^{ikx}}{2 \operatorname{ch}(k/2)} \partial \widehat{\ln(1+y_2)}(k) \quad (4.21)$$

$$= \partial \ln \Lambda_g(x) - \pi \int_{-\infty}^{\infty} \frac{dy}{2} \frac{\operatorname{sh}(\pi(x-y))}{\operatorname{ch}^2(\pi(x-y))} \ln(1+y_2)(y) \quad . \quad (4.22)$$

The expression can be used for asymptotics $y_k^\infty > 1$ (i.e. $\operatorname{ch} \phi \geq 1$) and opposite signs of the boundary fields $\alpha^\pm = \pm i(n^\pm/2 + \alpha^{\pm'})$ with $0 < \alpha^{\pm'} < 1/2$ and $n^\pm \in \mathbb{N}_0$ fixed.³ However, a change of the sign of one α -parameter transforms $\phi \rightarrow \phi \pm i\pi$ but leaves the asymptotics y_k^∞ from (4.19) unchanged. This again reflects the invariance of the functional equation (4.20) with respect to $\Lambda \rightarrow -\Lambda$ and $\alpha^\pm \rightarrow -\alpha^\pm$. As a remark the polynomial eigenvalue $\Lambda(\lambda)$ can be evaluated explicitly in the limit of $\phi \rightarrow \infty$ reading

$$\Lambda(\lambda) = \frac{(-1)^L \operatorname{ch} \phi}{\alpha^+ \alpha^-} (\lambda^2 + 1/4)^{L+1} \quad . \quad (4.23)$$

Note that the prefactor is recovered from the asymptotic behaviour (2.21) and does not contain the combined limit of $\phi, |\alpha^\pm| \rightarrow \infty$ but $\operatorname{ch} \phi / (\alpha^+ \alpha^-)$ fixed. Continuing (4.21) and (4.22) respectively to $x = i/2$ leaves us with the energy eigenvalue of the hamiltonian (1.1)

$$E = i\partial \ln \Lambda(i/2) = i\partial \ln \Lambda_g(i/2) - \pi \int_{-\infty}^{\infty} \frac{dy}{2} \frac{\operatorname{ch}(\pi y)}{\operatorname{sh}^2(\pi y)} \ln(1+y_2)(y) \quad . \quad (4.24)$$

The bulk and boundary part $E_g \equiv i\partial \ln \Lambda_g(i/2)$ was already specified in (2.23) and remains valid for any boundary conditions and all $0 < |\alpha^\pm| < \infty$ as the poles emerging from $0 < |\alpha^\pm| < 1/2$ in both $\Lambda(\lambda)$ and $\Lambda_g(\lambda)$ cancel out. Corrections due to correlations between the boundaries in the finite system are covered by the second term yielding the energy dependence in Figure 4. Clearly in the limit $\phi \rightarrow \infty$ the expression (4.23) diverges when the energy is calculated and reveals all hole-type solutions to accumulate at $\lambda = \pm i/2$.

5 Summary and Outlook

In this paper we have presented two approaches for the analysis of the functional equation describing the spectrum of the XXX spin chain with non-diagonal open boundary conditions (1.1). Based on the integrable structures underlying this model the TQ -equation arise both from Sklyanin's separation of variables and from the fusion procedure for transfer matrices. Usually, the solution of the TQ -equation for lattice models with compact realization of the symmetry can be re-expressed in terms of algebraic Bethe equations which are obtained in

³ In our derivation of the non-linear integral equations (4.18) we have restricted the boundary fields by choosing $n^+ = n^-$. In numerical solutions of the equations we find, however, that the error due to the violation of this constraint is of similar order as the one arising from the truncation of the infinite hierarchy, see Figure 4.

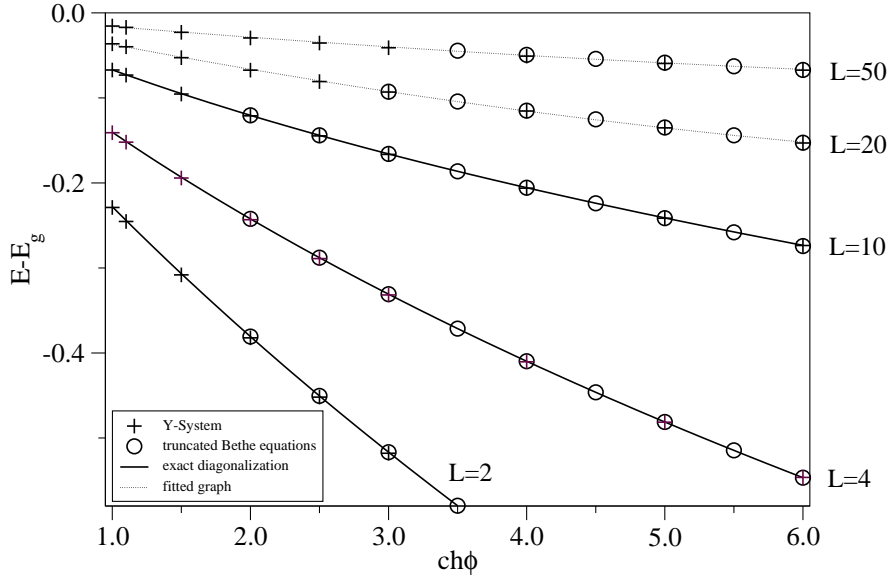


Figure 4: Influence of non-diagonal boundaries on the finite size effects to the energy eigenvalue for the A -state with parameters $\alpha^+ = 5i/3$ and $\alpha^- = -7i/5$ of different sign and lattice sizes $L = 2, 4, 10, 20, 50$. For large asymptotics $\text{ch } \phi$ the calculations are performed with the truncated Bethe equations (\circ) matching for intermediate values of $\text{ch } \phi$ the results from the Y -system ($+$). The latter one deals with low asymptotics down to $\text{ch } \phi = 1$. Solid lines are data from exact diagonalization for small system sizes $L = 2, 4, 10$.

a straightforward way starting with a polynomial ansatz for the Q -functions. For generic boundary conditions such an ansatz does not satisfy the requirements on the asymptotic behaviour of the eigenvalues in the present case (see [1, 9]). Starting from a finite size study of the analytic behaviour of the transfer matrix eigenvalues we have been able to express the functional equation in a way which opens the possibility of a numerical treatment for systems sizes beyond what is accessible to exact diagonalization. Both the truncated Bethe equations derived in Section 3 and the non-linear integral equations presented in Section 4 can be applied to compute the spectrum for non-diagonal boundary fields parametrized by $\text{ch } \phi > 1$. They are particularly useful to compute the energy of the state which evolves into the antiferromagnetic ground state of the chain for diagonal boundary conditions (the A -state).

The truncated Bethe equations are found to work especially well for $\text{ch } \phi \gg 1$ and can deal with arbitrary boundary parameters α^\pm . Going to large system sizes the numerical analysis of the equations is limited in principle by the necessity to find appropriate starting values for the Bethe roots. Still, selected energies can be computed for systems of several thousand sites. In the second method of non-linear integral equations the system size enters merely as a parameter. At the same time, however, boundary parameters α^\pm have to be of different sign to meet certain analyticity requirements. In addition, the presence of zeros together with the exponential growth of the asymptotic value of the y -functions with the level k leads to numerical instabilities limiting the use of these equations to boundary fields with $\text{ch } \phi = \mathcal{O}(1)$. Taken together the two methods are complementary allowing to cover

the entire range of boundary parameters with $\text{ch } \phi > 1$. Our numerical data show these approaches agree for intermediate values of $\text{ch } \phi$. Further support for their validity comes from comparison with exact diagonalization for lattices with up to 14 sites.

At the same time there remain several open problems which we shall address in the future: for the XXX chain (1.1) considered in this paper the description of the root distribution for the state evolving into the fully polarized ferromagnetic state in the limit of diagonal boundary conditions (B -state, see Figure 2) needs to be modified to extend the non-linear integral equations approach to this state. The limitation of the non-linear integral equations for the A -state to boundary parameters satisfying $\text{ch } \phi \gtrsim 1$ appears to be a technical problem which could be resolved eventually by finding an exact truncation of the infinite hierarchy of equations similar to that for the $sl(2)$ model [26]. Furthermore, the case $0 < \text{ch } \phi < 1$ corresponding to Hermitian boundary terms in (1.1) is not covered by our present approaches. An extension to this range of parameters may be possible following the treatment of excited states for the periodic XXZ chain to deal with hole-type solutions in the complex strip to be considered for the Y -System [13]. Similarly, the present restriction to opposite signs of the α -parameters in the non-linear integral equation approach could be resolved. Finally, the methods introduced here should be extended to the XXZ chain with non-diagonal boundaries. The corresponding TQ -equations have already been derived from the fusion procedure [29]. Of particular interest in this model is the expansion of the energy eigenvalues around the Bethe ansatz solvable case, $\text{ch } \phi = 1$, which would allow for a non-perturbative study of current fluctuations in certain models for diffusion in one dimension [6, 8].

Acknowledgements. The authors would like to thank F.H.L. Essler, A.M. Grabinski and A. Klümper for helpful discussions. This work has been supported by the Deutsche Forschungsgemeinschaft under grant numbers FR 737/6 and SE 1742/1-2. JHG acknowledges support from the NTH School for Contacts in Nanosystems.

A Asymptotic Truncation

As the system of equations (4.18) has alternating driving terms we assume two limiting functions $g_1(x)$ and $g_2(x)$ to truncate the system by

$$y_k(x) = y_k^\infty \frac{\tanh^2 |\pi x/2| g_1(x)}{b_k^{n^+}(x) b_k^{n^-}(x)} \quad , \quad y_{k'}(x) = y_{k'}^\infty \frac{\tanh^2 |\pi x/2| g_2(x)}{b_{k'}^{n^+}(x) b_{k'}^{n^-}(x)} \quad (\text{A.1})$$

for successive k and $k' = k + 1 \gg \max\{n^+, n^-\}$ supported by numerical observations. Inserting these into (4.18) we obtain two coupled non-linear integral equations

$$\begin{aligned} \ln g_1(x) &= s * \ln \left(\frac{1 + y_{k-1}^\infty \frac{b_1^0 g_2}{b_{k-1}^{n^+} b_{k-1}^{n^-}}}{1 + y_{k-1}^\infty} \cdot \frac{1 + y_{k+1}^\infty \frac{b_1^0 g_2}{b_{k+1}^{n^+} b_{k+1}^{n^-}}}{1 + y_{k+1}^\infty} \right) \\ \ln g_2(x) &= s * \ln \left(\frac{1 + y_{k'-1}^\infty \frac{b_1^0 g_1}{b_{k'-1}^{n^+} b_{k'-1}^{n^-}}}{1 + y_{k'-1}^\infty} \cdot \frac{1 + y_{k'+1}^\infty \frac{b_1^0 g_1}{b_{k'+1}^{n^+} b_{k'+1}^{n^-}}}{1 + y_{k'+1}^\infty} \right) \quad . \end{aligned} \quad (\text{A.2})$$

In the limit of $k \rightarrow \infty$ the coupled system linearizes due to the exponentially fast growing asymptotics y_k^∞ into

$$\begin{aligned}\ln g_1(x) &= 2s * \ln g_2 + 2s * \ln b_1^0 - 2s * \ln b_{k-1}^{n^+} - 2s * \ln b_{k-1}^{n^-} \\ \ln g_2(x) &= 2s * \ln g_1 + 2s * \ln b_1^0 - 2s * \ln b_{k'-1}^{n^+} - 2s * \ln b_{k'-1}^{n^-}\end{aligned}\tag{A.3}$$

and is solvable in Fourier space after differentiating to apply the residue theorem. The explicit expression reads

$$g_1(x) = \left[2 \operatorname{ch}(\pi x) \frac{\operatorname{ch}(\pi x/2)}{d_k^{n^+}(x)} \frac{\operatorname{ch}(\pi x/2)}{d_k^{n^-}(x)} \right]^2, \quad g_2(x) = \left[2 \operatorname{ch}(\pi x) \frac{\operatorname{ch}(\pi x/2)}{d_{k+1}^{n^+}(x)} \frac{\operatorname{ch}(\pi x/2)}{d_{k+1}^{n^-}(x)} \right]^2 \tag{A.4}$$

leaving the asymptotic of $y_k(x)$ unchanged as $g_{1/2}(x) \rightarrow 1$ for $x \rightarrow \pm\infty$ with the shorthands

$$d_k^n(x) = \begin{cases} \operatorname{ch}(\pi x) + \cos(\pi \alpha') & \text{for } n+k \text{ even} \\ \operatorname{ch}(\pi x) + \sin(\pi \alpha') & \text{for } n+k \text{ odd} \end{cases} . \tag{A.5}$$

References

- [1] L. Amico, H. Frahm, A. Osterloh, and T. Wirth, *Separation of variables for integrable spin-boson models*, Nucl. Phys. B **839** [FS] (2010), 604.
- [2] P. Baseilhac and K. Koizumi, *Exact spectrum of the XXZ open spin chain from the q -Onsager algebra representation theory*, J. Stat. Mech. (2007), P09006.
- [3] R. J. Baxter, *Exactly solved models in statistical mechanics*, Dover New York, 2008.
- [4] H. Bethe, *Zur Theorie der Metalle. I. Eigenwerte und Eigenfunktionen der linearen Atomkette*, Z. Phys. **71** (1931), 205.
- [5] A. G. Bytsko and J. Teschner, *On the spectrum of the sinh-Gordon model*, J. Phys. A: Math. Gen. **39** (2006), 12927.
- [6] J. de Gier and F. H. L. Essler, *Exact spectral gaps of the asymmetric exclusion process with open boundaries*, J. Stat. Mech. (2006), P12011.
- [7] H. J. de Vega and A. González-Ruiz, *Boundary K -matrices for the six vertex and the $n(2n-1)A_{n-1}$ vertex models*, J. Phys. A: Math. Gen. **26** (1993), L519.
- [8] B. Derrida, B. Douçot, and P.-E. Roche, *Current fluctuations in the one-dimensional symmetric exclusion process with open boundaries*, J. Stat. Phys. **115** (2004), 717.
- [9] H. Frahm, A. Seel, and T. Wirth, *Separation of variables in the open XXX chain*, Nucl. Phys. B **802** [FS] (2008), 351.

- [10] W. Galleas, *Functional relations from the Yang-Baxter algebra: Eigenvalues of the XXZ model with non-diagonal twisted and open boundary conditions*, Nucl. Phys. B **790** [PM] (2008), 524.
- [11] S. Ghoshal and A. Zamolodchikov, *Boundary S-matrix and boundary state in two-dimensional integrable quantum field theory*, Int. J. Mod. Phys. A **9** (1994), 3841, hep-th/9306002.
- [12] A. Klümper, *Integrability of quantum chains: Theory and applications to the spin-1/2 XXZ chain*, Quantum magnetism, Lecture notes in Physics, vol. 645, Springer Verlag Berlin, 2004, p. 349.
- [13] A. Klümper, J. R. Reyes Martínez, C. Scheeren, and M. Shiroishi, *The spin-1/2 XXZ chain at finite magnetic field: Crossover phenomena driven by temperature*, J. Stat. Phys. **102** (2000), 937.
- [14] A. Klümper and P. A. Pearce, *Conformal weights of RSOS lattice models and their fusion hierarchies*, Physica A **183** (1992), 304.
- [15] P. P. Kulish, *Yang-Baxter equation and reflection equations in integrable models*, Preprint, hep-th/9507070, 1995.
- [16] A. Kuniba, T. Nakanishi, and J. Suzuki, *Functional relations in solvable lattice models: I. functional relations and representation theory*, Int. J. Mod. Phys. A **9** (1994), 5215.
- [17] L. Mezincescu and R. I. Nepomechie, *Fusion procedure for open chains*, J. Phys. A: Math. Gen. **25** (1992), 2533.
- [18] R. Murgan, R. I. Nepomechie, and C. Shi, *Boundary energy of the open XXZ chain from new exact solutions*, Ann. H. Poincaré **7** (2006), 1429.
- [19] R. I. Nepomechie, *Solving the open XXZ spin chain with nondiagonal boundary terms at roots of unity*, Nucl. Phys. B **622** [FS] (2002), 615.
- [20] ———, *Bethe ansatz solution of the open XXZ chain with nondiagonal boundary terms*, J. Phys. A: Math. Gen. **37** (2004), 433.
- [21] S. Niekamp, T. Wirth, and H. Frahm, *The XXZ model with anti-periodic twisted boundary conditions*, J. Phys. A: Math. Theor. **42** (2009), 195008.
- [22] A. Seel and T. Wirth, *Non-linear integral equations and determinant formulae of the open XXZ spin chain*, J. Phys. A: Math. Theor. **42** (2009), 115202.
- [23] E. K. Sklyanin, *The quantum Toda chain*, Non-linear Equations in Classical and Quantum Field Theory, Lecture notes in Physics, vol. 226, Springer Verlag Berlin, 1985, p. 196.
- [24] ———, *Boundary conditions for integrable quantum systems*, J. Phys. A: Math. Gen. **21** (1988), 2375.

- [25] ———, *Nankai lectures in mathematical physics*, Quantum group and Quantum Integrable Systems, World Scientific, 1992, p. 63, hep-th/9211111.
- [26] J. Suzuki, *Spinons in magnetic chains of arbitrary spins at finite temperatures*, J. Phys. A: Math. Gen. **32** (1999), 2341.
- [27] M. Takahashi, *One-dimensional Heisenberg model at finite temperature*, Prog. Theor. Phys. **46** (1971), 401.
- [28] ———, *Thermodynamics of One-Dimensional Solvable Models*, Cambridge University Press, 1999.
- [29] W.-L. Yang, R. I. Nepomechie, and Y.-Z. Zhang, *Q-operator and T-Q relation from the fusion hierarchy*, Phys. Lett. B **633** (2006), 664.
- [30] Y. Zhou, *Fusion hierarchy and finite-size corrections of $U_q[sl(2)]$ -invariant vertex models with open boundaries*, Nucl. Phys. B **453** [FS] (1995), 619.
- [31] ———, *Row transfer matrix functional relations for Baxter's eight-vertex and six-vertex models with open boundaries via more general reflection matrices*, Nucl. Phys. B **458** [FS] (1996), 504.